

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

Model Results

Predicted value: 5.03e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 4.53e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>Mephosfolan</div> <div>Measured: 2.12e-04</div> <div>Predicted: 1.19e-03</div> | <div>Image not found</div> <div>Phosfolan</div> <div>Measured: 2.55e-03</div> <div>Predicted: 4.10e-03</div>  | <div>Image not found</div> <div>Naled</div> <div>Measured: 5.25e-03</div> <div>Predicted: 8.25e-03</div> |
| <div>Image not found</div> <div>Heptenophos</div> <div>Measured: 9.97e-03</div> <div>Predicted: 1.20e-02</div> | <div>Image not found</div> <div>Fosthietan</div> <div>Measured: 2.07e-01</div> <div>Predicted: 3.47e-02</div> |  |